2,3,4-TRICHLORO-1-BUTENE

Inchi: InChI=1S/C4H5Cl3/c1-3(6)4(7)2-5/h4H,1-2H2
InchiKey: WZUZDBPJFHQVJC-UHFFFAOYSA-N
Formula: C4H5Cl3
SMILES: C=C(Cl)C(Cl)CCl
Mol. weight [g/mol]: 159.44
CAS: 2431-50-7

Physical Properties

Property code	Value	Unit	Source
hfus	12.59	kJ/mol	Joback Method
logp	2.585		Crippen Method
mcvol	99.640	ml/mol	McGowan Method
tf	259.33	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.34	J/mol×K	399.33	Joback Method
cpg	156.00	J/mol×K	433.22	Joback Method
cpg	162.27	J/mol×K	467.11	Joback Method
cpg	168.14	J/mol×K	501.00	Joback Method
cpg	173.65	J/mol×K	534.90	Joback Method
cpg	178.81	J/mol×K	568.79	Joback Method
cpg	183.64	J/mol×K	602.68	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.61929e+02

Coeff. B	-3.22086e+04
Coeff. C	-9.89376e+01
Coeff. D	9.37238e-05
Temperature range (K), min.	303.15
Temperature range (K), max.	403.15

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1748

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pvap: Vapor pressure

tf: Normal melting (fusion) point